AD-A038 951 WISCONSIN UNIV MADISON MATHEMATICS RESEARCH CENTER F/G 12/1
AN EVALUATION PROCEDURE FOR INCOMPLETE GAMMA FUNCTIONS.(U)
FEB 77 W GAUTSCHI DAAG29-75-C-0024
UNCLASSIFIED MRC-TSR-1717 NL

1 OF 1
AD A038951

END
DATE FILMED
5-77

MRC Technical Summary Report #1717

AN EVALUATION PROCEDURE FOR INCOMPLETE GAMMA FUNCTIONS

Walter Gautschi

Mathematics Research Center
University of Wisconsin—Madison
610 Walnut Street
Madison, Wisconsin 53706

February 1977

(Received January 20, 1977)

Approved for public release
Distribution unlimited

Sponsored by

U. S. Army Research Office
P. O. Box 12211
Research Triangle Park
North Carolina 27709

National Science Foundation
Washington, D. C.
20550

UNIVERSITY OF WISCONSIN - MADISON
MATHEMATICS RESEARCH CENTER

AN EVALUATION PROCEDURE FOR INCOMPLETE GAMMA FUNCTIONS

Walter Gautschi

Technical Summary Report #1717
February 1977

ABSTRACT

We develop a computational procedure, based on Taylor's series and continued fractions, for evaluating Tricomi's incomplete gamma function $\gamma^*(a,x) = \frac{x^{-a}}{\Gamma(a)} \int_0^x e^{-t} t^{a-1} dt$ and the complementary incomplete gamma function $\Gamma(a,x) = \int_x^\infty e^{-t} t^{a-1} dt$, both in the region $x \geq 0$, $-\infty < a < \infty$.

AMS (MOS) Subject Classifications: 33-04, 33A15, 65D20

Key Words: computation of incomplete gamma functions, Taylor's series, continued fractions

Work Unit Number 7 (Numerical Analysis)

Sponsored by the United States Army under Contract No. DAAG29-75-C-0024 and the National Science Foundation under grant MCS 76-00842.

AN EVALUATION PROCEDURE FOR INCOMPLETE GAMMA FUNCTIONS

Walter Gautschi

1. Introduction. The incomplete gamma function, and its complementary function, are usually defined by

$$\gamma(a,x) = \int_0^x e^{-t}t^{a-1}dt, \quad \Gamma(a,x) = \int_x^\infty e^{-t}t^{a-1}dt . \tag{1.1}$$

By Euler's integral for the gamma function,

$$\gamma(a,x) + \Gamma(a,x) = \Gamma(a) . \tag{1.2}$$

We are interested in computing both functions for arbitrary x, a in the half-plane

$$\mathcal{H} = \{(x,a) : x \geq 0, \ -\infty < a < \infty\} .$$

The function $\Gamma(a,x)$ is meaningful everywhere in $\mathcal{H}$, except along the negative a-axis, where it becomes infinite. The definition of $\gamma(a,x)$ is less satisfactory, inasmuch as it requires $a > 0$. The difficulty, however, is easily resolved by adopting Tricomi's version [11] of the incomplete gamma function,

$$\gamma^*(a,x) = \frac{x^{-a}}{\Gamma(a)}\gamma(a,x) , \tag{1.3}$$

which can be continued analytically into the entire (x,a)-plane, resulting in an entire function both in a and x,

$$\gamma^*(a,x) = \frac{e^{-x}M(1,a+1;x)}{\Gamma(a+1)} = \frac{M(a,a+1;-x)}{\Gamma(a+1)} , \tag{1.4}$$

where $M(a,b;z) = 1 + \frac{a}{b}\frac{z}{1!} + \frac{a(a+1)}{b(b+1)}\frac{z^2}{2!} + \cdots$ is Kummer's function. Moreover, $\gamma^*(a,x)$ is real-valued for a and x both real, in contrast to $\Gamma(a,x)$, which becomes complex for negative x.

Our objective, then, is to compute $\gamma^*(a,x)$ and $\Gamma(a,x)$ to any prescribed accuracy for arbitrary x, a in $\mathcal{H}$. We do not attempt here to compute $\gamma^*(a,x)$ for negative x, which

Sponsored by the United States Army under Contract No. DAAG29-75-C-0024 and the National Science Foundation under grant MCS 76-00842.

may well be a more difficult (but, fortunately, less important) task. We accomplish our task by selecting one of the two functions as primary function, to be computed first, and computing the other in terms of the primary function by means of

$$\Gamma(a,x) = \Gamma(a)\{1 - x^a \gamma^*(a,x)\}, \tag{1.5}$$

or

$$\gamma^*(a,x) = x^{-a}\{1 - \frac{\Gamma(a,x)}{\Gamma(a)}\}. \tag{1.6}$$

If $\gamma^*(a,x)$ is the primary function, we evaluate it either by Taylor's series, or by a little-known continued fraction due to Perron. For $\Gamma(a,x)$ we use exclusively the classical continued fraction of Legendre. Careful attention is required when a is very close (or equal) to a nonpositive integer, in which case (1.5) is not suitable for computation.

An evaluation procedure of the generality attempted here is likely to be of interest in many diverse areas of application. Widely-used special cases of $\gamma^*(a,x)$ or $\Gamma(a,x)$ include K. Pearson's form of the incomplete gamma function [8],

$$I(u,p) = (u\sqrt{p+1})^{p+1}\,\gamma^*(p+1, u\sqrt{p+1}),\quad u \geq 0,\ p > -1, \tag{1.7}$$

the χ^2-probability distribution functions

$$P(\chi^2|\nu) = (\tfrac{1}{2}\chi^2)^{\nu/2}\,\gamma^*(\tfrac{\nu}{2}, \tfrac{1}{2}\chi^2),\quad Q(\chi^2|\nu) = \frac{1}{\Gamma(\frac{\nu}{2})}\,\Gamma(\tfrac{\nu}{2}, \tfrac{1}{2}\chi^2), \tag{1.8}$$

the exponential integrals

$$E_\nu(x) = x^{\nu-1}\Gamma(-\nu+1, x) \tag{1.9}$$

(which, for $\nu = -n$, a negative integer, yield the molecular integrals $A_n(x)$ [5]), and the error functions

$$\operatorname{erf} x = x\gamma^*(\tfrac{1}{2}, x^2),\quad \operatorname{erfc} x = \frac{1}{\sqrt{\pi}}\,\Gamma(\tfrac{1}{2}, x^2). \tag{1.10}$$

When a is integer-valued, $\gamma^*(a,x)$ becomes an elementary function,

$$\gamma^*(-n,x) = x^n,\quad \gamma^*(n+1,x) = x^{-(n+1)}[1 - e^{-x}e_n(x)],\quad n = 0,1,2,\ldots, \tag{1.11}$$

where $e_n(x) = \sum_{k=0}^{n} x^k/k!$.

2. Asymptotic formulas. It is useful to have some general idea as to the magnitude of the functions $\Gamma(a,x)$ and $\gamma^*(a,x)$, when one or both variables are large. If a is bounded, and $x \to \infty$, it is well known [12, p. 174] that

$$\Gamma(a,x) \sim e^{-x}x^{a-1}, \quad x \to \infty, \quad |a| \text{ bounded}. \tag{2.1}$$

By (1.6), this implies

$$\gamma^*(a,x) \sim x^{-a}, \quad x \to \infty, \quad |a| \text{ bounded}. \tag{2.2}$$

Equally simple is the case $|x|$ bounded and $a \to \infty$ (over positive values of a), in which case [12, p. 175]

$$\gamma^*(a,x) \sim \frac{e^{-x}}{\Gamma(a+1)}, \quad a \to \infty, \quad |x| \text{ bounded}, \tag{2.3}$$

hence, by (1.5),

$$\Gamma(a,x) \sim \Gamma(a), \quad a \to \infty, \quad |x| \text{ bounded}. \tag{2.4}$$

An indication of the behavior, when both variables are large, can be gained by setting $x = \rho a$, $\rho > 0$ fixed, and letting $a \to \infty$. Laplace's method, applied to the integrals in (1.1), then gives

$$\Gamma(a,\rho a) \sim \begin{cases} \Gamma(a), & 0 < \rho < 1, \\ \frac{1}{2}\Gamma(a), & \rho = 1, \\ \frac{(a\rho)^a e^{-a\rho}}{(1+\rho)a}, & \rho > 1, \end{cases} \qquad a \to \infty, \tag{2.5}$$

and

$$\gamma^*(a,\rho a) \sim \begin{cases} \frac{e^{-a\rho}}{(1-\rho)\Gamma(a+1)}, & 0 < \rho < 1, \\ \frac{1}{2}a^{-a}, & \rho = 1, \\ (\rho a)^{-a}, & \rho > 1, \end{cases} \qquad a \to \infty. \tag{2.6}$$

Similarly,

$$\Gamma(-a,\rho a) \sim \frac{(a\rho)^{-a}e^{-a\rho}}{(1+\rho)a}, \quad 0 < \rho < \infty, \quad a \to \infty, \tag{2.7}$$

from which, by (1.6) and the reflection formula for the gamma function,

$$\gamma^*(-a, \rho a) \sim \begin{cases} \dfrac{\sin \pi a}{(1+\rho)\pi}\,\Gamma(a)e^{-a\rho} & \text{if } \rho e^{1+\rho} < 1, \quad a \neq 0 \pmod 1, \\ (\rho a)^a & \text{if } \rho e^{1+\rho} \geq 1, \end{cases} \qquad a \to \infty. \tag{2.8}$$

Uniform asymptotic expansions are derived in [10].

3. Choice of primary function. We recall from (1.5), (1.6) that either of the two functions $\Gamma(a,x)$, $\gamma^*(a,x)$ can be expressed in terms of the other by means of

$$\Gamma(a,x) = \Gamma(a)\{1 - x^a\gamma^*(a,x)\}, \quad \gamma^*(a,x) = x^{-a}\{1 - \frac{\Gamma(a,x)}{\Gamma(a)}\}. \tag{3.1}$$

In our choice of primary function, we are guided by two considerations: the numerical stability of (3.1), and computational convenience.

With regard to numerical stability, we must be careful not to loose excessively in accuracy when we perform the subtractions indicated in curled brackets in (3.1). No such loss occurs if the absolute value of the respective difference is larger than, or equal to, $\frac{1}{2}$. This criterion is easily expressed in terms of the ratio

$$r(a,x) = \frac{\Gamma(a,x)}{\Gamma(a)}. \tag{3.2}$$

Indeed, the first relation in (3.1) is stable exactly if $|r(a,x)| \geq \frac{1}{2}$, while the second is stable in either of the two cases $r(a,x) \geq \frac{3}{2}$ and $r(a,x) \leq \frac{1}{2}$. As a consequence, an ideal choice of the primary function is $\gamma^*(a,x)$ if $\frac{1}{2} \leq r(a,x) \leq \frac{3}{2}$, and $\Gamma(a,x)$ if $|r(a,x)| \leq \frac{1}{2}$; in all remaining cases either choice is satisfactory.

For the practical implementation of this criterion, consider first $a > 0$, $x > 0$. In this case, $0 < r(a,x) < 1$, and $r(a,x)$ increases monotonically in the variable a ([11, p. 276]). Since $\lim_{a \to 0} r(a,x) = 0$ and, by (2.4), $\lim_{a \to \infty} r(a,x) = 1$, there is a unique curve $a = \rho(x)$ in the first quadrant $x > 0$, $a > 0$, along which $r(a,x) = \frac{1}{2}$, and $r(a,x) \gtrless \frac{1}{2}$ depending on whether $a \lessgtr \rho(x)$. Since, by (2.5), $r(x,x) \sim \frac{1}{2}$ as $x \to \infty$, we have $\rho(x) \doteq x$ for x large. By numerical computation it is found that in fact $\rho(x) \doteqdot x$ for all positive x, the value of $\rho(x)$ consistently being slightly larger than x. Ideally, a good choice for the primary function then is $\Gamma(a,x)$ if $0 < a < x$, and $\gamma^*(a,x)$ if $a \geq x > 0$.

Direct computation of $\Gamma(a,x)$, when a and x are both relatively small, however, is difficult, owing to the singular behavior of $\Gamma(a,x)$ near $a = 0$, $x = 0$. In contrast,

$\gamma^*(a,x)$ is easily computable from its Taylor series, when x is small and a is arbitrary. These practical considerations lead us to choose $\Gamma(a,x)$ as primary function only if $x > 1.5$ and $a < x$, while $\gamma^*(a,x)$ is taken as primary function in all other cases. The choice of the breakpoint $x = 1.5$ is further motivated in Section 5.2.

An analogous discussion in the case $a < 0$, $x > 0$ is complicated by the more involved behavior of $r(a,x)$, and also by the presence of lines along which $\gamma^*(a,x)$ vanishes. Computational convenience, nevertheless, dictates the same choices of primary functions, as made above in the case $a > 0$, $x > 0$. Thus, if we divide the half-plane $\mathcal{H}$ into three regions as shown in Figure 3.1, labelled I, II, III, we use $\gamma^*(a,x)$ as primary function in regions I and II, and $\Gamma(a,x)$ in region III. The partition of Figure 3.1 also reflects different choices of computing methods: Taylor's series for $\gamma^*(a,x)$ in region I, Perron's continued fraction in region II, and Legendre's continued fraction in region III.

Since practical considerations led us to deviate from the ideal choice of primary function, some loss of accuracy will be unavoidable. The problem is most pronounced in region I when a is close to a nonpositive integer. It also occurs in the lower portion of region III near zero-curves of $\gamma^*(a,x)$. The simplest remedy, in most cases, consists in computing the primary and secondary function in double precision (when available). An exception to this arises in region I, when a is very close (or equal!) to a nonpositive integer, in which case we need to compute the appropriate limit function. This is further discussed in Section 5.

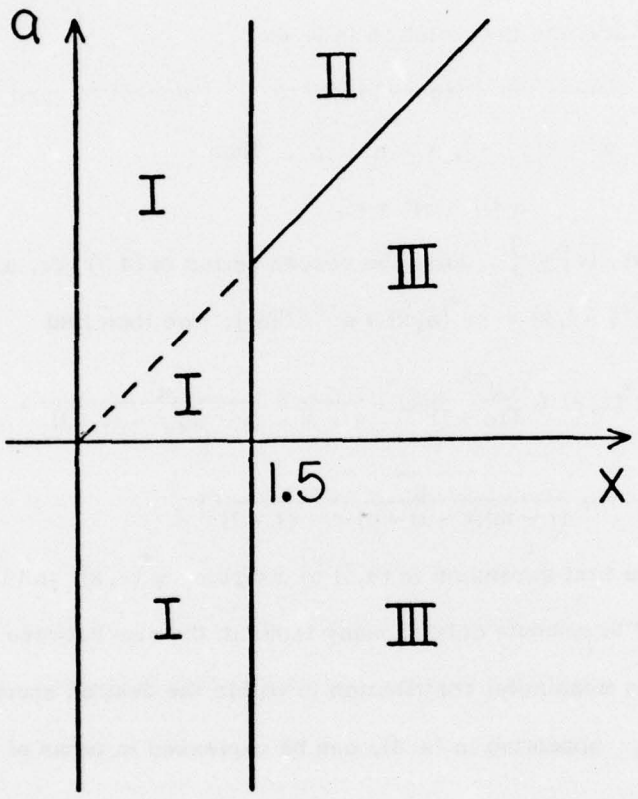

Fig. 3.1. Partition of domain $\mathcal{X}$

4. Taylor's series for $\gamma^*(a,x)$. The following series expansions follow immediately from (1.4),

$$\gamma^*(a,x) = \frac{1}{\Gamma(a+1)} \sum_{n=0}^{\infty} \frac{a(-x)^n}{(a+n)n!} = e^{-x} \sum_{n=0}^{\infty} \frac{x^n}{\Gamma(a+n+1)} . \tag{4.1}$$

When $a \geq -\frac{1}{2}$, we prefer the first expansion, since it terminates after the first term when $a = 0$. Although the series is alternating, its sum is always positive (in fact, larger than e^{-x}) when $a > -1$, as is seen from the first relation in (1.4).

If $a < -\frac{1}{2}$, we let $\{a\}$ denote the integer closest to a [closest to, and less than, a, in case of a tie], and define $m = -\{a\} - 1$, $\epsilon = a - \{a\}$. Then

$$a + 1 = -m + \epsilon ,$$

where $m \geq 0$ is an integer, and $|\epsilon| \leq \frac{1}{2}$. From the second series in (4.1) [or, alternatively, from the recurrence relation $\gamma^*(a-1,x) = x\gamma^*(a,x) + e^{-x}/\Gamma(a)$], we then find

$$\gamma^*(a,x) = x^{m+1}\gamma^*(\epsilon,x) + \frac{e^{-x}}{\Gamma(a+1)} \{1 + \frac{x}{\epsilon - m} + \frac{x^2}{(\epsilon - m)(\epsilon - m + 1)} + \cdots + \frac{x^m}{(\epsilon - m)(\epsilon - m + 1)\cdots(\epsilon - 1)}\} . \tag{4.3}$$

Since $|\epsilon| \leq \frac{1}{2}$, we can use the first expansion in (4.1) to compute $\gamma^*(\epsilon,x)$ in (4.3). Also, when m is very large, we need to compute only as many terms in the sum between curled brackets as are required to give a meaningful contribution to within the desired accuracy.

The reciprocal of $\Gamma(a+1)$, appearing in (4.3), can be expressed in terms of m and ϵ as

$$\frac{1}{\Gamma(a+1)} = (-1)^m \frac{\epsilon\,\Gamma(m+1-\epsilon)}{\Gamma(1+\epsilon)\Gamma(1-\epsilon)} . \tag{4.4}$$

By virtue of $m \geq 0$, $|\epsilon| \leq \frac{1}{2}$, this requires an evaluation routine for $\Gamma(x)$ that needs to be effective only in the range $x \geq \frac{1}{2}$. It should be noted, however, that when a is very close to a negative integer, ϵ will be small and inaccurate, causing the evaluation in (4.4) to be inaccurate.

5. Evaluation of $\Gamma(a,x)$ when a is near a nonpositive integer. Special analysis is required for $\Gamma(a,x)$ when a is very close to a nonpositive integer, and $0 < x \leq 1.5$. The primary function then is $\gamma^*(a,x)$, and Equation (1.5) expresses $\Gamma(a,x)$ as a product of two quantities, one very large in absolute value, and the other very small - the difference of two almost equal numbers. Computationally, this is unsatisfactory and can lead to gross inaccuracies. If $m \geq 0$ is an integer, however, it is known that

$$\Gamma(-m,x) = x^{-m}E_{m+1}(x), \quad x > 0 , \tag{5.1}$$

where $E_{m+1}(x)$ is the exponential integral of order $m+1$ (cf. [1, Eq. 5.1.4]). It is of interest, therefore, to discuss under what conditions the right-hand side of (5.1) is an acceptable approximation to $\Gamma(a,x)$, when $a \doteq -m$, and how to compute $x^{-m}E_{m+1}(x)$.

5.1. Limit behavior of $\Gamma(a,x)$ as $a \to -m$. Consider

$$\Gamma(-m+\epsilon,x) = \int_x^\infty e^{-t}t^{-m+\epsilon-1}dt, \quad x > 0 ,$$

where $m \geq 0$ is an integer, and $|\epsilon|$ is small, say, $|\epsilon| \leq \frac{1}{2}$. We have

$$\Gamma(-m+\epsilon,x) = \int_x^\infty e^{-t}\{t^{-m-1} + t^{-m-1}(t^\epsilon - 1)\}dt = x^{-m}E_{m+1}(x) + \int_x^\infty e^{-t}t^{-m-1}(t^\epsilon - 1)dt ,$$

so that

$$\Gamma(-m+\epsilon,x) - x^{-m}E_{m+1}(x) = \int_x^\infty e^{-t}t^{-m-1}(t^\epsilon - 1)dt .$$

Using Taylor's theorem, we have

$$t^\epsilon = e^{\epsilon \ell nt} = 1 + e^{\theta\epsilon \ell nt} \cdot \epsilon \ell nt, \quad \theta = \theta(\epsilon,t), \quad 0 < \theta < 1 ,$$

giving

$$\Gamma(-m+\epsilon,x) - x^{-m}E_{m+1}(x) = \epsilon \int_x^\infty e^{-t}t^{-m-1}e^{\theta\epsilon \ell nt}\ell nt\, dt . \tag{5.2}$$

We consider first the case $0 < x < 1$. Since

$$e^{\theta\epsilon \ell nt} \le e^{-|\epsilon|\ell nt} = t^{-|\epsilon|}, \quad \text{if} \quad 0 < t < 1,$$

and

$$\ell nt \le t - 1, \quad \text{if} \quad t \ge 1,$$

we obtain for the integral in (5.2),

$$\left| \int_x^\infty \cdots dt \right| \le \int_x^1 e^{-t} t^{-m-1} t^{-|\epsilon|} |\ell nt| dt + \int_1^\infty e^{-t} t^{-m-1} t^{|\epsilon|} (t-1) dt \tag{5.3}$$

$$\le x^{-|\epsilon|} |\ell nx| x^{-m} E_{m+1}(x) + \int_1^\infty e^{-t} t^{-m} (t-1) dt .$$

The integral on the far right equals e^{-1} if $m = 0$, $e^{-1} - E_1(1)$ if $m = 1$, and $E_{m-1}(1) - E_m(1)$ if $m \ge 2$. Using the inequalities ([1, Eq. 5.1.19])

$$\frac{e^{-x}}{x+n} < E_n(x) \le \frac{e^{-x}}{x+n-1}, \quad x > 0, \quad n = 1, 2, 3, \ldots, \tag{5.4}$$

we find

$$\int_1^\infty e^{-t} t^{-m} (t-1) dt \le \alpha_m e^{-1}, \quad \alpha_m = \begin{cases} 1 & \text{if} \quad m = 0, \\ \frac{1}{2} & \text{if} \quad m = 1, \\ \frac{2}{m^2 - 1} & \text{if} \quad m \ge 2, \end{cases}$$

and therefore, by (5.2) and (5.3),

$$\left| \frac{\Gamma(-m+\epsilon, x) - x^{-m} E_{m+1}(x)}{x^{-m} E_{m+1}(x)} \right| \le |\epsilon| \left\{ x^{-|\epsilon|} |\ell nx| + \frac{\alpha_m e^{-1}}{x^{-m} E_{m+1}(x)} \right\} .$$

Since $x^{-m} E_{m+1}(x) = \Gamma(-m, x)$ clearly decreases, as x increases, we have, again with the help of (5.4),

$$x^{-m} E_{m+1}(x) > E_{m+1}(1) > \frac{e^{-1}}{m+2}, \quad 0 < x < 1,$$

and thus, finally,

$$(5.5)\qquad \left|\frac{\Gamma(-m+\epsilon,x)-x^{-m}E_{m+1}(x)}{x^{-m}E_{m+1}(x)}\right| \le |\epsilon|\{x^{-|\epsilon|}|\ell nx| + (m+2)\alpha_m\}, \quad 0<x<1,$$

where

$$(5.6)\qquad (m+2)\alpha_m = \begin{cases} 2 & \text{if } m=0, \\ \frac{3}{2} & \text{if } m=1, \\ \frac{2(m+2)}{(m+1)(m-1)} & \text{if } m\ge 2. \end{cases}$$

In the case $x \ge 1$, we estimate the integral in (5.2) by

$$\left|\int_x^\infty \cdots dt\right| \le \int_x^\infty e^{-t}t^{-m-1}|\epsilon|_{\ell nt}\, dt \le \int_x^\infty e^{-t}t^{-m}(t-1)dt,$$

from which

$$\left|\frac{\Gamma(-m+\epsilon,x)-x^{-m}E_{m+1}(x)}{x^{-m}E_{m+1}(x)}\right| \le \frac{|\epsilon|}{x^{-m}E_{m+1}(x)}\int_x^\infty e^{-t}t^{-m}(t-1)dt.$$

The integral on the right evaluates to xe^{-x} if $m=0$, to $e^{-x}-E_1(x)$ if $m=1$, and to $x^{-(m-2)}E_{m-1}(x) - x^{-(m-1)}E_m(x)$ if $m\ge 2$. Using once more the inequalities in (5.4), we find

$$(5.7)\qquad \left|\frac{\Gamma(-m+\epsilon,x)-x^{-m}E_{m+1}(x)}{x^{-m}E_{m+1}(x)}\right| \le |\epsilon| \cdot \begin{cases} x(x+1) & \text{if } m=0, \\ \frac{x^2(x+2)}{x+1} & \text{if } m=1, \\ x(x+m+1)\{\frac{x}{x+m-2}-\frac{1}{x+m}\} & \text{if } m\ge 2. \end{cases}$$

If we restrict attention to the interval $1 \le x \le 1.5$, the factor of $|\epsilon|$ in (5.7) can be bounded, respectively, by $\frac{15}{4} = 3.75$, $\frac{63}{20} = 3.15$, and $\frac{135}{28} = 4.821\ldots$, so that

$$(5.8)\qquad \left|\frac{\Gamma(-m+\epsilon,x)-x^{-m}E_{m+1}(x)}{x^{-m}E_{m+1}(x)}\right| \le 5|\epsilon|, \quad 1\le x\le 1.5.$$

Since the approximation $x^{-m}E_{m+1}(x)$ will only be used if $|\epsilon|$ is quite small, we shall assume, somewhat arbitrarily, that $|\epsilon| \le .001$. Then $x^{-m}E_{m+1}(x)$ approximates $\Gamma(-m+\epsilon,x)$ correctly to d significant decimal places, whenever

$$|\epsilon|\{x^{-.001}|\ell nx| + (m+2)\alpha_m\} \le \tfrac{1}{2}10^{-d}, \quad 0 < x < 1,$$

$$5|\epsilon| \le \tfrac{1}{2}10^{-d}, \quad 1 \le x \le 1.5. \tag{5.9}$$

5.2. Evaluation of $x^{-m}E_{m+1}(x)$. We propose to use the expansion [1, Eq. 5.1.12]

$$x^{-m}E_{m+1}(x) = \frac{(-1)^m}{m!}\left\{-\ell nx + \psi(m+1) + \frac{x}{m+1}\sum_{r=0}^{\infty}\frac{(-x)^r(m+1)!}{(r+1)(m+1+r)!}\right\} + \frac{x^{-m}}{m}\sum_{s=0}^{m-1}\frac{(-x)^s m}{s!(m-s)}, \tag{5.10}$$

where the last term is understood to be zero if $m = 0$, and where

$$\psi(m+1) = -\gamma + \sum_{k=1}^{m}\frac{1}{k},$$

$\gamma = .5772...$ being Euler's constant. It is important to make sure that little cancellation take place among the various terms on the right of (5.10). Empirical computations convinced us that no more than approximately one decimal digit is lost due to cancellation, if we restrict x to the interval $[0,1.5]$, the cancellation being noticeable only near $x = 1.5$ when $m = 0,1,2$ or 3. This, in fact, is one of the motivations for placing the break at $x = 1.5$ in the partition of Figure 3.1. (Another motivation is the progressively slower convergence of Legendre's continued fraction for $\Gamma(a,x)$ as x decreases.)

Assuming, then, $0 < x \le 1.5$, it is easily verified that all partial sums of the infinite series in (5.10), as well as the sum itself, are strictly positive. Since, moreover, $-\ell nx + \psi(m+1) \ge -\ell n\, 1.5 + \psi(2) = -.4054... + .4227... > 0$ for $m \ge 1$, we see that the expression between curled brackets in (5.10) is also positive for $m \ge 1$. No such statement can be made for the finite series in (5.10), which can be negative, zero, or positive. Its terms, when m is large, need to be computed only so long as they contribute significantly.

6. Legendre's continued fraction for $\Gamma(a,x)$. The following continued fraction, due to Legendre, is well-known ([9, p. 103], [1, Eq. 6.5.31]),

$$x^{-a}e^{x}\Gamma(a,x) = \frac{1}{x+}\,\frac{1-a}{1+}\,\frac{1}{x+}\,\frac{2-a}{1+}\,\frac{2}{x+}\cdots . \tag{6.1}$$

It converges for any $x > 0$ and for arbitrary real a. We can write (6.1) in contracted form as

$$x^{-a}e^{x}\Gamma(a,x) = \frac{\beta_0}{x+\alpha_0+}\,\frac{\beta_1}{x+\alpha_1+}\,\frac{\beta_2}{x+\alpha_2+}\cdots ,$$

$$\alpha_k = 2k+1-a, \quad k = 0,1,2,\ldots ,$$

$$\beta_0 = 1, \ \beta_k = k(a-k), \quad k = 1,2,3,\ldots ,$$

or, alternatively, in the form

$$(x+1-a)x^{-a}e^{x}\Gamma(a,x) = \frac{1}{1+}\,\frac{a_1}{1+}\,\frac{a_2}{1+}\,\frac{a_3}{1+}\cdots , \tag{6.2}$$

where

$$a_k = \frac{k(a-k)}{(x+2k-1-a)(x+2k+1-a)}, \quad k = 1,2,3,\ldots . \tag{6.3}$$

We investigate the convergence character of the continued fraction in (6.2) for $-\infty < a \le x$, $x \ge 1.5$, which is the region III in Figure 3.1, where (6.2) is going to be used.

It is well-known (cf., e.g., [13, p. 17ff]) that any continued fraction of the form (6.2) can be evaluated as an infinite series,

$$\frac{1}{1+}\,\frac{a_1}{1+}\,\frac{a_2}{1+}\,\frac{a_3}{1+}\cdots = \sum_{k=0}^{\infty} p_k , \tag{6.4}$$

where

$$p_0 = 1, \ p_k = \rho_1\rho_2\cdots\rho_k, \quad k = 1,2,3,\ldots , \tag{6.5}$$

$$\rho_0 = 0, \ \rho_k = \frac{-a_k(1+\rho_{k-1})}{1+a_k(1+\rho_{k-1})}, \quad k = 1,2,3,\ldots . \tag{6.6}$$

The n-th partial sum in (6.4), in fact, is equal to the n-th convergent of the continued fraction, $n = 1, 2, 3, \ldots$. If we let

$$\sigma_k = 1 + \rho_k ,$$

then the recursion for ρ_k in (6.6) translates into the following recursion for σ_k,

$$\sigma_0 = 1, \quad \sigma_k = \frac{1}{1 + a_k \sigma_{k-1}}, \quad k = 1, 2, 3, \ldots . \tag{6.7}$$

Consider now the case of a_k as given in (6.3). If $k < a$ (thus $a > 1$), then $a_k > 0$ (since $a \leq x$), and it follows inductively from (6.7) that $0 < \sigma_k < 1$, hence $-1 < \rho_k < 0$. In view of (6.5), this means that (6.4) initially behaves like an alternating series with terms decreasing monotonically in absolute value.

If $k > a$, then $a_k < 0$, and σ_k may become larger than one. However, if $0 < \sigma_{k-1} \leq 2$, we claim that $1 < \sigma_k \leq 2$ whenever $x \geq \frac{1}{4}$. Indeed, for the upper bound we must show that $1 + a_k \sigma_{k-1} \geq \frac{1}{2}$, i.e., $a_k \sigma_{k-1} \geq -\frac{1}{2}$, or, equivalently, $|a_k| \sigma_{k-1} \leq \frac{1}{2}$. Since $\sigma_{k-1} \leq 2$, it suffices to show $|a_k| \leq \frac{1}{4}$, which is equivalent to $1 \leq (x - a)^2 + 4kx$. Since $k \geq 1$ and $x > 0$, the latter is certainly true if $x \geq \frac{1}{4}$, which proves the assertion $\sigma_k \leq 2$. The other inequality, $1 < \sigma_k$, is an easy consequence of $1 + a_k \sigma_{k-1} > 0$, established in the course of the argument just given, and the negativity of a_k. Since for the first k with $k > a$ we have $0 < \sigma_{k-1} \leq 1$ (by virtue of the discussion in the preceding paragraph, or by virtue of $\sigma_0 = 1$), it follows inductively that $1 < \sigma_k \leq 2$ for all $k > a$, hence $0 < \rho_k \leq 1$. In the case $k = a$, we have $a_k = 0$ and $\sigma_k = 1$, thus $\rho_k = 0$, and the argument again applies.

We have shown that $|\rho_k| \leq 1$ for all $k \geq 1$, that is, the terms in the series of (6.4) are nonincreasing in modulus, whenever $-\infty < a \leq x$, $x \geq \frac{1}{4}$, in particular, therefore, when (x, a) is in the region III of Figure 3.1. Moreover, the series changes from an alternating series, initially, to a monotone series, ultimately.

In the region $a > x$, convergence of Legendre's continued fraction may deteriorate considerably in speed, which, together with the appropriate choice of primary function, is the reason why we prefer Perron's continued fraction for $a > x$ (cf. Section 7).

7. Perron's continued fraction for $\gamma^*(a,x)$. From the differential equation satisfied by Kummer's function $M(a,b;z)$, Perron [9, p. 278] derives the following continued fraction,

$$\frac{M(a+1,b+1;z)}{M(a,b;z)} = \frac{b}{b-z+}\ \frac{(a+1)z}{b+1-z+}\ \frac{(a+2)z}{b+2-z+}\ \cdots . \tag{7.1}$$

We have shown in [2] that, when $z = -x < 0$ and $0 < a + 1 \le b$, the continued fraction (7.1) converges monotonically in the sense that all convergents are positive and increase monotonically to their limit. Letting $b = a + 1$, and taking note of the second relation in (1.4), we find immediately

$$\frac{\gamma^*(a+1,x)}{\gamma^*(a,x)} = \frac{1}{a+1+x-}\ \frac{(a+1)x}{a+2+x-}\ \frac{(a+2)x}{a+3+x-}\ \cdots ,$$

which may be combined with $x\gamma^*(a+1,x) = \gamma^*(a,x) - e^{-x}/\Gamma(a+1)$ to yield

$$\Gamma(a+1)e^x\gamma^*(a,x) = \frac{1}{1-\varphi}, \quad \varphi = \frac{x}{a+1+x-}\ \frac{(a+1)x}{a+2+x-}\ \frac{(a+2)x}{a+3+x-}\ \cdots . \tag{7.2}$$

The algorithm in (6.4) - (6.6) may be used to evaluate φ, if we write

$$\frac{a+1+x}{x}\,\varphi = \frac{1}{1+}\ \frac{a_1}{1+}\ \frac{a_2}{1+}\ \frac{a_3}{1+}\ \cdots , \tag{7.3}$$

with

$$a_k = -\frac{(a+k)x}{(a+k+x)(a+k+1+x)}, \qquad k = 1,2,3,\ldots . \tag{7.4}$$

Perron's continued fraction in (7.2) will be used only for $a \ge x \ge 1.5$, i.e., in region II of Figure 3.1.

The speed of convergence increases with a, hence is slowest when $a = x$. Compared to Legendre's continued fraction (6.1), Perron's continued fraction unfortunately converges only about half as fast near the line $a = x$. This is illustrated in Table 7.1, which shows the number of convergents required for relative accuracies $\frac{1}{2}10^{-d}$, $d = 8(4)20$, Legendre's continued fraction (L) being used for $a = .999x_r$, Perron's continued fraction (P) for $a = 1.001x_r$, where $x_r = .3872 + 5(r-1)$, $r = 5(5)40$.

d	r	5	10	15	20	25	30	35	40
	x_r	20.3872	45.3872	70.3872	95.3872	120.3872	145.3872	170.3872	195.3872
8	L	15	20	24	27	29	31	33	34
	P	29	40	49	55	61	66	71	76
12	L	18	25	30	34	37	40	42	44
	P	38	53	64	73	81	88	94	100
16	L	20	30	36	40	44	47	50	52
	P	46	64	77	88	97	106	113	121
20	L	22	34	41	46	50	54	57	60
	P	54	74	89	101	112	122	130	139

Table 7.1. Speed of convergence of Legendre's (L) and Perron's (P) continued fraction near the line $a = x$.

Equation (7.2) is subject to a potential loss of accuracy when $\varphi \doteq 1$. From the asymptotic results in Section 2, however, we can see that $\varphi \to 0$ when x is fixed and $a \to \infty$. When $x = \rho a$ and ρ is fixed in $0 < \rho \leq 1$, then $\varphi \to \rho$ as $a \to \infty$. Any significant cancellation, therefore, appears to be possible only near the line $x = a$, when a is large. Even then, however, the problem is very minor, since $\gamma^*(a,a) \sim \frac{1}{2} a^{-a}$, hence $1 - \varphi = 1 - \sqrt{\frac{2}{\pi a}}\,(1 + o(1))$, as $a \to \infty$. We thus loose between one and two decimal digits only if $a \doteq 640$, at which point $\gamma^*(a,a) \doteq 10^{-1800}$, much too small to be representable on most computers.

8. Flowchart. We briefly review the salient features of the complete evaluation procedure, which forms the basis of the algorithm in [3], and encapsulate them in the flowchart of Figure 8.1 below.

Our goal is to evaluate $\gamma^*(a,x)$ and $\Gamma(a,x)$ to d correct significant decimal places, where $d \le d_0$, with d_0 denoting the number of decimal digits available on the computing device at hand. (On a binary computer with β binary digits in the mantissa of the single-precision floating-point word, we may set $d_0 = \beta \ell n 2 / \ell n 10$.) Due to unavoidable rounding errors, and the possibility of minor cancellation errors at a few places (e.g., in Taylor's series for the exponential integral and in Perron's continued fraction; cf. Section 5.2 and the final paragraph of Section 7), it would be unrealistic to require $d = d_0$. We shall in fact tolerate losses of 1 to 2 decimal digits, before taking any precautions, so that a reasonable choice of d should be less than $d_0 - 1$ or $d_0 - 2$.

Due to our choice of primary function (cf. Section 3), more serious cancellation errors may be incurred in the use of

$$\Gamma(a,x) = \Gamma(a)\{1 - x^a \gamma^*(a,x)\} \tag{8.1}$$

when $0 < x \le 1.5$ and $a \le x$, and in the use of

$$\gamma^*(a,x) = x^{-a}\left\{1 - \frac{\Gamma(a,x)}{\Gamma(a)}\right\} \tag{8.2}$$

when $x > 1.5$ and $a < 0$. With regard to (8.2), the problem is only significant near a zero of $\gamma^*(a,x)$. In our algorithm in [3] we make no attempt at achieving full significant accuracy near zero-curves of $\gamma^*(a,x)$. Instead, we issue an appropriate message to the user of the algorithm, if the accuracy requirement cannot be met.

In (8.1), the loss of accuracy is most prominent when a is close to a nonpositive integer,

$$a \doteq -m, \qquad m = 0, 1, 2, \ldots .$$

Different actions are taken, in this instance, depending on whether double-precision is available or not. If it is, we recompute the expression on the right of (8.1) in double precision,

whenever the single-precision calculation (to d digits!) reveals that

$$|1 - x^a \gamma^*(a,x)| \le .05 , \tag{8.3}$$

i.e., when the d-digit accuracy in $\Gamma(a,x)$ is in jeopardy. If single precision is the only precision mode available, and if enough extra precision is available (say, $10^{d_0-d} > 20$), the occurrence of (8.3) will prompt us to recompute $\Gamma(a,x)$ to full single-precision accuracy. If these countermeasures prove to be of no avail, then again our algorithm issues an appropriate message. This will notably be the case if

$$|1 - x^a \gamma^*(a,x)| \le 10^{-(d_0-d)} , \tag{8.4}$$

after γ^* has been recomputed to an accuracy of d_0 decimal digits.

It is possible to estimate how close to a nonpositive integer $-m$ the value of a has to be for the predicament (8.4) to occur. From (8.2), and $\Gamma(-m,x) = x^{-m}E_{m+1}(x)$, it follows indeed that

$$\gamma^*(a,x) = x^m - [x^m \ell nx + (-1)^m m! E_{m+1}(x)]\epsilon + O(\epsilon^2), \quad \epsilon = a + m \to 0 ,$$

from which

$$1 - x^a \gamma^*(a,x) = (-1)^m m! x^{-m} E_{m+1}(x)\epsilon + O(\epsilon^2), \quad \epsilon \to 0 .$$

Neglecting the $O(\epsilon^2)$-term, we thus have (8.4) if

$$m! x^{-m} E_{m+1}(x)|\epsilon| \le 10^{-(d_0-d)} ,$$

which, by virtue of $x^{-m}E_{m+1}(x) \ge 1.5^{-m}E_{m+1}(1.5)$, implies

$$|\epsilon| \le \kappa_m 10^{-(d_0-d)} , \quad \kappa_m = \frac{1}{m!\,1.5^{-m}E_{m+1}(1.5)} . \tag{8.5}$$

(The first few values of κ_m are: $\kappa_0 = 9.9980$, $\kappa_1 = 20.520$, $\kappa_2 = 19.827$, $\kappa_3 = 12.226$, $\kappa_4 = 5.4746$, $\kappa_5 = 1.9137, \ldots$.) Thus, for our procedure to concede defeat, the value of a must be sufficiently close to $-m$ so as to have (8.5), but not so close as to satisfy (5.9), since then the limit value (for $a \to -m$) will be accurate enough.

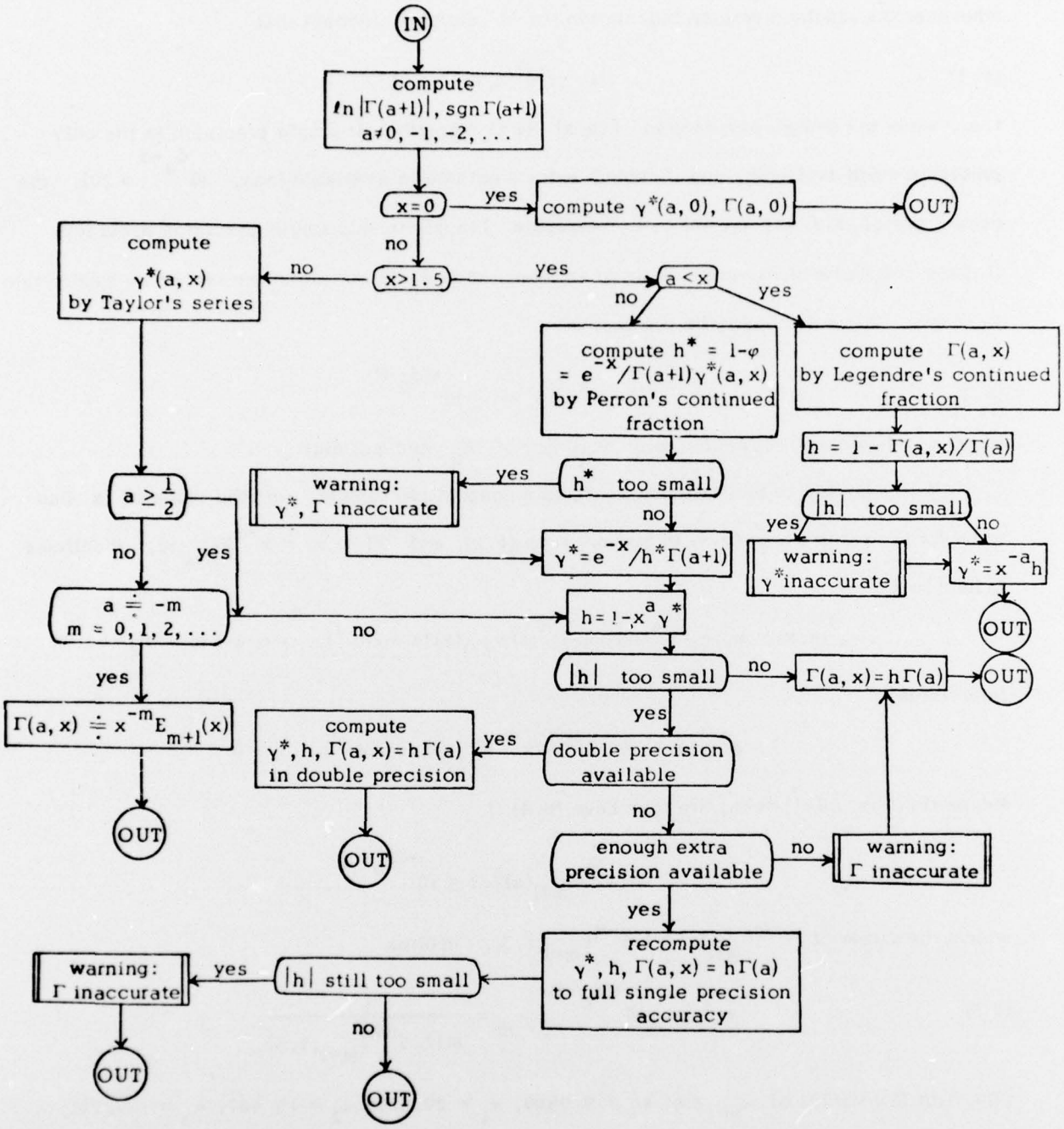

Figure 8.1. Flow chart for computing $\gamma^*(a, x)$ and $\Gamma(a, x)$

An important feature of our algorithm is the automatic monitoring of overflow and underflow conditions. This is accomplished by first computing the logarithm of the desired quantities and by making the tests for overflow and underflow on the logarithms. As a result, minor inaccuracies are introduced in the final exponentiation, particularly if the result is near the overflow or underflow limit.

9. Testing. The algorithm in [3], and a double-precision version of it, were tested extensively on the CDC 6500 computer at Purdue University and on the UNIVAC 1110 computer at the University of Wisconsin. The double-precision algorithm was used to provide reference values for checking the single-precision algorithm, and on a few occasions, to check against high-precision tables (notably the 14S tables in [6]). Other reference values were taken from various mathematical tables in the literature.

The tests include:

(i) the error functions (1.10), checked against Tables 7.1 and 7.3 in [1];

(ii) the case (1.11) of integer values $a = n$, $-20 \le n \le 20$;

(iii) the exponential integral $E_\nu(x)$ in (1.9) for integer values $\nu = n$, $0 \le n \le 20$, and fractional values of ν in $0 \le \nu \le 1$, checked against Tables I, II, III in [7];

(iv) Pearson's incomplete gamma function (1.7), checked against Tables I and II in [8];

(v) the incomplete gamma function $P(a,x) = (x/2)^a \gamma^*(a,x/2)$, checked against the tables in [4];

(vi) the χ^2-distribution (1.8), checked against Table 26.7 in [1];

(vii) the molecular integral $A_n(x)$, checked against Table 1 in [5] and the more accurate tables in [6].

In addition, the performance of the routines was examined for parameter values a in the neighborhood of zero and in the neighborhood of negative integers. When a is very close to a negative integer, the accuracy of $\gamma^*(a,x)$ was observed to deteriorate substantially. This is due to inaccuracies in the evaluation of $\Gamma(a+1)$, as remarked at the end of Section 4.

An important feature of our algorithm is the automatic monitoring of overflow and underflow conditions. This is accomplished by first computing the logarithm of the desired quantities and by making the tests for overflow and underflow on the logarithms. As a result, minor inaccuracies are introduced in the final exponentiation, particularly if the result is near the overflow or underflow limit.

References

[1] M. Abramowitz and I. A. Stegun (eds.), Handbook of Mathematical Functions, Nat. Bur. Standards Appl. Math. Series, Vol. 55 (1964).

[2] W. Gautschi, Anomalous convergence of a continued fraction for ratios of Kummer functions, to be published.

[3] W. Gautschi, Algorithm ... - Incomplete gamma functions, to be published.

[4] S. H. Khamis, Tables of the Incomplete Gamma Function Ratio, Justus von Liebig Verlag, Darmstadt, 1965.

[5] M. Kotani, A. Amemiya, E. Ishiguro and T. Kimura, Table of Molecular Integrals, Maruzen Co., Ltd., Tokyo, 1955.

[6] J. Miller, J. M. Gerhausen and F. A. Matsen, Quantum Chemistry Integrals and Tables, University of Texas Press, Austin, 1959.

[7] V. I. Pagurova, Tables of the exponential integral $E_\nu(x) = \int_1^\infty e^{-xu} u^{-\nu} du$. (Translated from the Russian by D. G. Fry) Pergamon Press, New York, 1961.

[8] K. Pearson (ed.), Tables of the Incomplete Γ-Function, Biometrika Office, University College, Cambridge University Press, Cambridge, England, 1934.

[9] O. Perron, Die Lehre von den Kettenbrüchen, Vol. II, 3rd ed., B. G. Teubner, Stuttgart, 1957.

[10] N. M. Temme, Uniform asymptotic expansions of the incomplete gamma functions and the incomplete beta function, Math. Comp. 29 (1975), 1109-1114.

[11] F. G. Tricomi, Sulla funzione gamma incompleta, Ann. Mat. Pura Appl. (4) 31 (1950), 263-279.

[12] F. G. Tricomi, Funzioni ipergeometriche confluenti, Edizioni Cremonese, Rome, 1954.

[13] H. S. Wall, Analytic Theory of Continued Fractions, D. van Nostrand Co., New York, 1948. {Reprinted in 1967 by Chelsea Publ. Co., Bronx, N. Y.}.

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER: MRC-TSR-1717	2. GOVT ACCESSION NO.
3. RECIPIENT'S CATALOG NUMBER: Technical	
4. TITLE (and Subtitle): AN EVALUATION PROCEDURE FOR INCOMPLETE GAMMA FUNCTIONS.	5. TYPE OF REPORT & PERIOD COVERED: Summary Report - no specific reporting period
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s): Walter Gautschi	8. CONTRACT OR GRANT NUMBER(s): DAAG29-75-C-0024; NSF-MCS-76-00842
9. PERFORMING ORGANIZATION NAME AND ADDRESS: Mathematics Research Center, University of Wisconsin, 610 Walnut Street, Madison, Wisconsin 53706	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: 7 (Numerical Analysis)
11. CONTROLLING OFFICE NAME AND ADDRESS: See Item 18 below.	12. REPORT DATE: February 1977
	13. NUMBER OF PAGES: 23
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office): 28p.	15. SECURITY CLASS. (of this report): UNCLASSIFIED
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

U. S. Army Research Office
P. O. Box 12211
Research Triangle Park
North Carolina 27709

National Science Foundation
Washington, D. C.
20550

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

computation of incomplete gamma functions
Taylor's series
continued fractions

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

We develop a computational procedure, based on Taylor's series and continued fractions, for evaluating Tricomi's incomplete gamma function

$$\gamma^*(a,x) = \frac{x^{-a}}{\Gamma(a)} \int_0^x e^{-t} t^{a-1}\,dt$$

and the complementary incomplete gamma function

$$\Gamma(a,x) = \int_x^\infty e^{-t} t^{a-1}\,dt,$$

both in the region $x \geq 0$, $-\infty < a < \infty$.

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

221200